

We are pleased to welcome Pam Esposito to the Protein Data Bank staff. Pam works part time and is handling all data distributions. With the additional volume of new data, orders, and associated recordkeeping, Pam's assistance to the Data Bank is especially valuable.

Because of the increased number of coordinate entries included in DATAPRTP, we anticipate that shortly we will no longer be able to include all entries on two tapes at 1600 cpi. We strongly encourage users to switch over to ordering 6250 cpi tapes as soon as possible.

As was announced in the April Newsletter (Number 44), on-line access to DATAPRTP is being provided by the Canadian Scientific Numeric Data Base Service (CAN/SND) in Ottawa (contact Dr. Roger S. Gough, telephone 613-993-3294, Electronic Mail CANSND@NRCVM01) and the Pittsburgh Supercomputing Center (contact Dr. Hugh B. Nicholas, telephone 412-268-4960, Electronic Mail NICHOLAS@CPWPSCA).

The established Protein Data Bank centers continue to provide their full range of services. Inquiries may be addressed as shown below. The order form on pages 5-6 of this newsletter may be used to order data from Brookhaven. It is possible to place a standing order for each quarterly DATAPRTP release; anyone interested in placing such a standing order should contact F. C. Bernstein. Please note that the order form on pages 5-6 should be used only for Brookhaven orders; users in Japan or Australia should contact their centers for detailed information.

Area	Address of Center	BITNET (BNL Only)	Name	Phone
Worldwide except Australia and Japan	Protein Data Bank	PDB@BNLCHM	Inquiries	516-282-4382
	Chemistry Department	ABOLA@BNLCHM	E. E. Abola	516-282-4383
	Brookhaven National Laboratory	BERNSTEIN@BNLCHM	F. C. Bernstein	516-282-4382
	Upton, NY 11973	BRYANT@BNLCHM	P. A. Esposito	516-282-4382
	USA	KOETZLE@BNLCHM	S. H. Bryant	516-282-4375
		WENG@BNLCHM	T. F. Koetzle	516-282-4384
			J. C. Weng	516-282-4382
Australia	CSIRO Division of Biotechnology 343 Royal Parade, Parkville Victoria 3052, Australia		P. Davis	03-342-4326
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2 Suita, Osaka 565, Japan		Y. Katsube	(06) 877-5111 ext. 3912

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TABLE 1. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE

CODE	ITEM	16-JUL-88		
		USA	JAP	AUS
DATAPRTP	ALL CURRENT COORDINATE ENTRIES (TABLE 5), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 7 - NO COORDINATES IN BIB ENTRIES)	X	X	X
YEARS77P	NEW OR REVISED COORDINATE ENTRIES FOR 1987	X		
PART88TP	NEW OR REVISED COORDINATE ENTRIES FOR 1988 (TO DATE)	X		
PDBPGMTP	COMPUTER PROGRAMS AND MISCELLANEOUS FILES (TABLE 3, PARTS A AND B)	X		
NONST1TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 1)	X	X	
NONST2TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 2)	X	X	
NONST3TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 3)	X	X	
NONST4TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 4)	X	X	
NONST5TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 5)	X	X	
NONST6TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 6)	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	X		
BLDKITTP	MODEL BUILDER'S KIT	X		
CONNECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X		
DGPIOTTP	DIAGONAL PLOTS (LINE PRINTER)	X		
DIDRLTTP	COMPLETE TORSION ANGLES	X		
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X		
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)	X		
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES	X		

* NEW OR REPLACEMENT ENTRY SINCE APR-88 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	16-JUL-88		
		USA	JAP	AUS
DATAPRFI	ALL CURRENT COORDINATE ENTRIES (TABLE 5), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 7 - NO COORDINATES IN BIB ENTRIES)	X	X	X
YEARS7FI	NEW OR REVISED COORDINATE ENTRIES FOR 1987	X		
PART88FI	NEW OR REVISED COORDINATE ENTRIES FOR 1988 (TO DATE)	X		
CORR22FI	*LIST OF CORRECTIONS NO. 22 (JAN/88 - JUL/88)	X	X	X
NONST1FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 1)	X	X	
NONST2FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 2)	X	X	
NONST3FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 3)	X	X	
NONST4FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 4)	X	X	
NONST5FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 5)	X	X	
NONST6FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 6)	X	X	
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X		
BLDKITFI	MODEL BUILDER'S KIT	X		
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X		
DGPIOTFI	DIAGONAL PLOTS (LINE PRINTER)	X		
DIDRLFI	COMPLETE TORSION ANGLES	X		
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X		
FISIPLFI	PHI/PSI PLOTS (LINE PRINTER)	X		
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X		

* NEW OR REPLACEMENT ENTRY SINCE APR-88 NEWSLETTER

Table with 4 columns: ID, Description, Depositor, Date/Status. Includes entries like 2RLX RELAXIN (CONFORMATION B, UNREFINED) MODEL A. EVANS, A. NORTH 3/78 P.

* NEW OR REPLACEMENT ENTRY SINCE APR-88 NEWSLETTER
STATUS CODES
BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
R RECENT (1986-1988) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET
TABLE 6. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION 16-JUL-88

Main table listing protein entries with columns: IDENT, MOLECULE, DEPOSITOR(S), DATE/STATUS. Includes entries like 5WGA *AGGLUTININ (WHEAT GERM, ISOLECTIN 2) C. WRIGHT 6/88 RP.

* NEW OR REPLACEMENT ENTRY SINCE APR-88 NEWSLETTER
STATUS CODES
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P IN PREPARATION
R REPLACEMENT FOR ENTRY IN TABLE 5
SF STRUCTURE FACTORS
TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES (NO COORDINATES) 16-JUL-88

Table listing protein entries with columns: ID, Description, Depositor, Date/Status. Includes entries like 0EAP ACID PROTEINASE (ENDOTHRIS PARASITICA) O.W.GI 1/88 SF.

Main table listing protein entries with columns: IDENT, MOLECULE, DEPOSITOR(S), DATE/STATUS. Includes entries like 0DN1 DEOXYRIBONUCLEASE I (DNASE I) OC3A DES-ARG77-C3A ANAPHYLATOXIN.

* NEW OR REPLACEMENT ENTRY SINCE APR-88 NEWSLETTER
TABLE 8. CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS 16-JUL-88

CORRECTIONS TO ENTRIES MAY BE OBTAINED IN ONE OF TWO WAYS -
A. ORDER CORR22FI. THERE IS NO CHARGE FOR THIS MICROFICHE WHICH CONTAINS A LISTING OF ALL CORRECTIONS APPLIED IN THE LAST SIX MONTHS.

B. ORDER A NEW COPY OF DATAPRTF.
THE FOLLOWING DATA SETS HAVE HAD CORRECTIONS APPLIED. PLEASE CONSULT A COPY OF THE PROTEIN DATA BANK ANNOTIC COORDINATE AND BIBLIOGRAPHIC ENTRY FORMAT DESCRIPTION FOR A FULL DESCRIPTION OF REV DAT RECORDS.

Table with 4 columns: ID, Date, Program, Count. Lists corrections for various programs like 9 16-APR-88 5LDBH 3 ATOM.

Table with 4 columns: ID, Old Entry, New Entry, Count. Lists replacements like OBSLTE 16-APR-88 2FD1 3FD1.

BROOKHAVEN ORDER FORM (Please include a self-addressed label)

1. Name _____ Date _____
 Address _____ Telephone _____
 _____ Electronic Mail _____

2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (April 1988)
 Latest Newsletter
 Atomic Coordinate and Bibliographic Entry Format Description
 for DATAPRTP and DATAPRFI (January 1985)
 Current DATAPRTP Directory
 Sources of Visual Aids for Macromolecular Structure (February 1988)
 Non-Standard Entries (Structure Factors) Format Description
 Data Deposition Form

3. Please send the following magnetic tape items (from Table 1).

	6250 cpi	1600 cpi	TK50
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	<input type="checkbox"/> \$283
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST5TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST6TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	

Cost: _____

Special order items (described in Table 1): Please inquire at Brookhaven for availability and price.

YEAR87TP	CONECTTP	DSTNCETP
PART88TP	DGPLOTP	FISIPLTP
BENDERTP	DIHDRLTP	PHIPSITP

(Continued)

4. Foreign air mail postage for tape items listed in 3 above mailed from Brookhaven to destinations outside the U.S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19 = _____

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$292, postage included. Correction fiche are free.

Items: _____ Cost: _____

6. Please send the following printed listings. Each listing costs \$95, postage included.

Ident Code(s) (From Table 5): _____ Cost: _____

7. Total charges - All prices are expected to be valid through September 30, 1988. After that date please confirm prices.

Magnetic tape charges (3 above) _____

Foreign air mail postage charges (4 above) _____

Microfiche charges (5 above) _____

Printed listing charges (6 above) _____

Bank charge _____

No charge for checks drawn in U.S. dollars on _____

U.S. bank, otherwise \$10 _____

TOTAL COST : _____

METHOD OF PAYMENT:

Brookhaven requires that either a written purchase order or check payable to

BROOKHAVEN NATIONAL LABORATORY

be received before service is provided. Order forms and purchase orders maybe sent by facsimile to (United States) 516-282-5815. The original order forms and purchase orders should also be sent to Brookhaven by mail.

() check is () enclosed
 () purchase order number _____ () sent separately

Please return ORDER FORM to

BROOKHAVEN NATIONAL LABORATORY
 Chemistry Department - Bldg. 555
 Ms. F. C. Bernstein
 Upton, New York 11973 USA
 (516-282-4382)

It is advisable to send a photocopy of this order form directly to Brookhaven; experience shows that purchasing departments often do not forward this form with the order.